Asymmetric exclusion processes with constrained dynamics

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Asymmetric exclusion processes with locally reversible kinetic constraints are introduced to investigate the effect of non-conservative driving forces in athermal systems. At high density they generally exhibit rheological-like behavior, negative differential resistance, two-step structural relaxation, dynamical heterogeneity and, possibly, a jamming transition driven by the external field.

There is a growing appreciation that glassy relaxation can be ascribed to purely dynamic restriction on the particle motion with static correlations and related thermodynamic factors playing little or no role [1, 2, 3]. Kinetically constrained models (KCMs) provide a simple and elegant way to rationalize this idea and have spurred the challenge to reproduce much of the observed glassy behavior [4], including detailed predictions that first originated in apparently unrelated and complementary mean-field approaches [5, 6]. While investigations of KCMs have been mostly focused on equilibrium and aging dynamics, there are relatively few studies dealing with the effects of nonconservative forces. The issue is of special interest in rheology, where the apparent viscosity of structured liquids is found to depend on the applied stirring force [7]. Shear-thinning refers to the commonly observed situations in which the viscosity decreases at increasing forces, and is well described by mode-coupling theory [8]. The opposite, shear-thickening, behavior is less common and much more difficult to predict. In some cases the viscosity increase can be so dramatic that the macroscopic motion may even stop, the liquid jams [7, 9]. It has been suggested that shear-thickening and jamming [10] are related to an underlying glass transition [11]. The idea has been interpreted microscopically in terms of an entropy-driven inverse freezing [12] and recent experiments have come to support this interpretation [13, 14]. The latter approach, however, requires some special thermodynamic and structural features which are absent in athermal shear-thickening systems (e.g. concentrated suspensions of hard spheres). Accordingly, any attempt at unifying different types of dynamical arrest in systems dominated by steric hindrance and packing effects should explain the simultaneous emergence of thinning and thickening behavior with their underlying glassy dynamics.

In this Letter I will show that rheological-like behavior occurs in microscopic models of finite dimensional particle systems interacting only through non-Hamiltonian forces and purely kinetic constraints. Evidence is provided by considering a variant of the asymmetric simple exclusion process (ASEP) [15], in which particle motion obeys an additional constraint motivated by lattice glass models [16]. Similarly to the ASEP the transition probabilities satisfy local detailed balance although, due to the periodic boundary condition, the driving field cannot be derived from a Hamiltonian. The applied field induces a nonequilibrium steady state (NESS) in the system. At small field the transport is ohmic and thinning behavior is observed. At high density, due to the imposed kinetic restrictions on the particle motion, the ohmic regime shrinks and the current decreases at increasing field, a negative differential resistance effect. The system can thus be driven, at constant density, into a regime close to jamming in which the dynamics is slow but stationary. In this regime, shear-thickening and other salient features of glassy behavior like two-step relaxation and dynamical heterogeneities are observed.

The model. ASEP describes a 1D lattice model of hard-core particles hopping randomly to a vacant nearest-neighbour site with rates $p_\pm$ depending on the direction of the particle move. Current-carrying NESSs are maintained either by fixing periodic boundary conditions, or by connecting the open boundaries to two particle-reservoirs at different densities. In the latter form the ASEP was originally introduced to model the biopolymerization kinetics on nucleic acid templates [17], and has come to play a paradigmatic role in recent developments of nonequilibrium statistical mechanics [15, 18]. ASEP-type models have been also studied in relation to vehicular traffic, molecular motors and intra/extra-cellular transport [19].

In this work, a variant of the 2D ASEP with discrete-time evolution is introduced in which particle hopping occurs with probability $p = \min\{1, \exp{(\vec{E} \cdot \vec{dr})}\}$, where $\vec{E}$ is the applied field and $\vec{dr}$ is the displacement unit vector, provided that an additional condition is met: the particle is constrained to have a number of neighboring particles below a certain threshold both before and after the move [16]. The constraint is naturally inspired by the cage effect in viscous liquids and leads to glassy relaxation at high density. In zero field, one recovers the boundary-driven constrained diffusion model of Ref. [20]. For periodic boundary conditions, the kinetic nature of the constraint guarantees that the equilibrium measure is trivial. The fully irreversible case is obtained in the opposite limit of infinite drive, corresponding to the kinetically constrained version of the totally asymmetric simple exclusion process.

For simplicity we consider square-lattice systems (of

size L^2) with periodic boundary conditions in which the driving force is applied along a lattice axis. The kinetic constraint is chosen to depend isotropically on the nearest neighbors with a threshold set to three. This constraint ensures that diffusion coefficient at equilibrium is finite at any nonzero vacancy [1]. Thus, no "true" glass transition is present in zero field although the dynamics is slow at high density and characterized by the cooperative motion of spatially extended mobility defects, whose size grows with the density [1]. For finite field, every allowed particle move in the direction opposite to the field can always occur with finite probability. This would imply that the irreducibility and ergodicity proofs given in Ref. [1] may be extended to the NESS, provided that the field intensity E is finite. Some technical steps, however, may be not straightforward because, in contrast with the equilibrium case and with the ASEP, the probability weight of constant-density configurations is nonuniform in the NESS, even though the average density profile is flat.

A first insight in the flow behavior can be gained by looking at the particle current J vs the driving force. At densities below $\rho \simeq 0.79$, J first grows linearly with E (ohmic regime) and then tends to saturate at large fields. This behavior is qualitatively similar to that observed in the ASEP and will not be further considered here. At densities above $\rho \simeq 0.79$ the transport properties differ rather markedly from the ASEP: the current shows a transition from the ohmic regime at small fields to a non-monotonic regime in which the current attains a maximum at finite field (rather than at saturation as in the previous case), and then decreases for larger field, see fig. 1. The region with negative slope in the "current-voltage" characteristics is traditionally known as incremental negative resistance (NR) and is a key ingredient in many biological systems and solid-state devices. Microscopic stochastic models yielding NR are known [20, 21]. In our case, NR does not depend on any static interaction and occurs because, at high density and increasing field, the particle rearrangements needed to remove obstruction to the flow, require more and more particle moves against, or normal to, the field direction (see, fig. 4c in Ref. [22] for an illustration). Three distinct behaviors may arise at high ρ:

I. Saturation current attains a finite (nonzero) value.

II. Saturation current vanishes.

III. Current vanishes at a finite driving force.

Numerical results suggest that regime I occurs in the range $0.79 < \rho < 0.83$ while regime II appears at higher density. For the present model, the ergodicity result mentioned above should prevent the existence of regime III in the thermodynamic limit, for large but finite E. Distinguishing between the two latter regimes, however, may be difficult due to the strong finite-size effects related
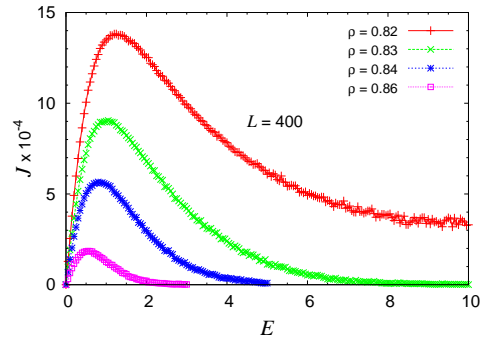

FIG. 1: Stationary current J vs field E at density ρ.

to bootstrap percolation [1, 2]. The characterization of these effects is notoriously difficult and will not be attempted here. Kinetic constraints having a more involved dependence on the neighboring particles [23, 24], will arguably have a jamming transition at finite field in the thermodynamic limit. Moreover, KCMs having single mobility defects may only have type-I behavior, no matter how large the particle density. This is confirmed by the behavior of a noncooperative driven KA model on triangular lattice.

NESS dynamics is expected to be slow in the NR region of high density as the current becomes vanishingly small at increasing forcing. This can be analyzed through the persistence function $\phi(t)$, i.e. the probability that the occupation variable of a lattice site has never changed between times 0 and t. The two stages responsible for equilibrium relaxation – which consist of particle rearrangements within spatially extended mobility defects and their subsequent coalescence [1] – are found to respond differently to the applied field.

At small field, relaxation under flow is slower than at equilibrium on short and intermediate time scales. At longer time scales, on the other hand, the macrodefects coalescence speeds up, and the relaxation behavior changes smoothly from a stretched to a simple exponential decay. The two stages of relaxation are well separated by a density-dependent crossover time, see fig. 2 (upper panel).

At large field, the thinning regime disappears because the time over which the first-stage relaxation occurs in the NESS exceeds the one required for the second-stage to take place in equilibrium. Consequently, ϕ develops a more marked two-step behavior in which the correlation decay becomes slower and slower at increasing field. The resulting thickening-like behavior is shown in the lower panel of fig. 2. The late stage relaxation in this regime obeys the superposition principle, $\phi(t) = \Phi(t/\tau_{\rm rel}(\rho, E))$, where the scaling function Φ is a simple exponential for the model under consideration, and $\tau_{\rm rel}(\rho, E) = \int_0^\infty \phi(t)dt$ is the integrated relaxation
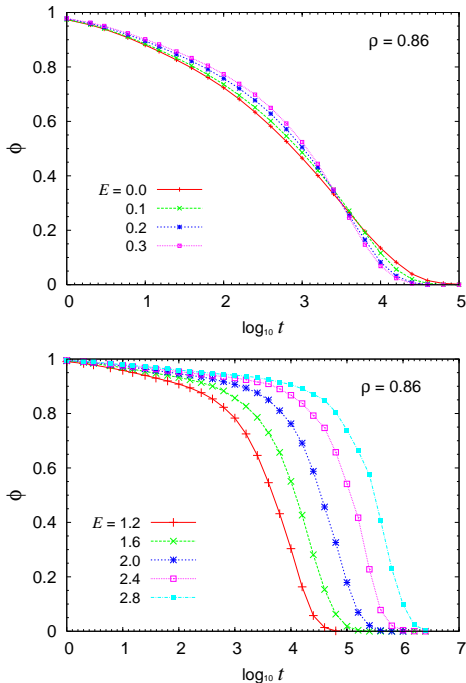
FIG. 3: Integrated relaxation time τ_{rel} vs driving force E.

FIG. 2: Steady state persistence ϕ vs time t at density ρ, for small (upper panel) and large (lower panel) applied field E.

time. τ_{rel} is a measure of the system viscosity and encodes the overall relaxation resulting from the superposition of the two above-mentioned competing effects. Fig. 3 clearly shows that at large enough density, τ_{rel} first decreases at small field and then increases (exponentially) at large field. To better appreciate the result above one should consider that outside the linear response regime the "resistivity" E/J increases with E, while the relaxation time is roughly independent of E at low density. This confirms that viscosity (rather than "resistivity") does generally account for the genuine flow properties of our model. The nonmonotonic dependence of viscosity at high density and the related transition from thinning to thickening behavior, are features observed in sheared hard-sphere suspensions [7]. In fact, flow curve analogs, obtained by identifying the shear stress with E and the shear rate with $E/\tau_{\mathrm{rel}}(\rho, E)$, are similar to those found in the "Model II" of the schematic mode-coupling theories studied in [11]. In this case, since kinetic constraints are "hard", no fluidisation occurs after jamming no matter how strong the force may be. If violation of constraints is allowed at large field, however, one should recover the flow curves of "Model I" and "Model III" of Ref. [11].

Notice that in contrast with the nonmonotonic behavior of viscosity and current, the fraction of blocked particles increases with E, even when transport is ohmic. The driving force thus generally enhances the clustering of particles and appears to be akin to a static short-range attractio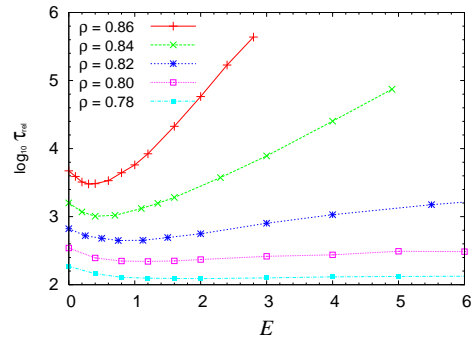n. In fact, models of this type do have a non-monotonic dependence of the relaxation time with the attraction strength at equilibrium [25]. This observation suggests an analogy between attraction-driven inverse freezing and shear-thickening/jamming.

Finally, dynamic heterogeneity in the NESS can be quantified by the fluctuations of persistence, $\chi_4(t) = N(\langle \phi^2(t) \rangle - \langle \phi(t) \rangle^2)$ where $N = \rho V$ [26, 27]. Similarly to equilibrium supercooled liquids [27] we find that dynamic heterogeneity and long range order grows with the applied field, as exemplified by the increasing peak in the dynamic susceptibility $\chi_4(t)$, and consistently with the monotonic increase of the fraction of blocked particle with E. However, in the thinning regime the peak occurs at shorter and shorter times as the field grows. In the thickening regime, on the other hand, the peak height and the time at which the peak occurs both increases with the applied field, as shown in fig. 4. Interestingly, even though the dynamics is obviously nonisotropic, the longitudinal and transverse persistence (and related fluctuations) are almost indistinguishable. Tiny differences only appear in the early stage of relaxation at large field. Thus, there is no substantial change in the corresponding longitudinal and transverse relaxation times.

Conclusions To summarize, when KCMs are driven into a nonequilibrium stationary state they show both an initial speed-up of the dynamics and then a pronounced slowdown at increasing fields. This suggests a common kinetic mechanism for the nonmonotonic viscosity of athermal systems and their thinning-thickening transition. The basic ingredient is the presence of two relaxation stages responding differently to the applied field. Such a behavior occurs in the simplest case of a spatially uniform nonconservative force. We expect that including a space dependent driving (to mimick more realistically a shear stress) yields similar results. In particular, the peculiar time evolution of dynamic heterogeneities observed here in the thinning and thickening regime should be experimentally accessible in sheared granular materials and concentrated colloidal suspensions. Finally, the existence of a jamming/blocking transition, possibly induced by
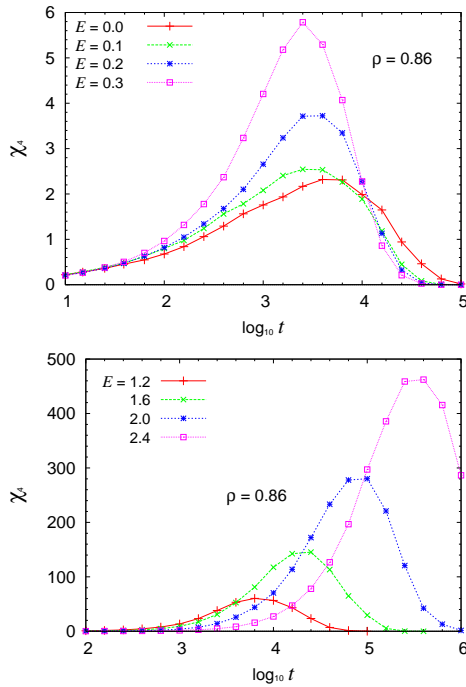
FIG. 4: Steady state four-point correlation χ_4 vs time t for small (upper panel) and large (lower panel) applied field E.

strong finite-size effects, implies that driven cooperative KCMs, are able to sustain indefinitely an applied stress above a certain threshold, and thus to provide a microscopic realization of *fragile matter* [28].

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